Key Role of Orbital Anisotropy in Geometrically Frustrated Electron System

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Abstract

By using the density matrix renormalization group method, we investigate ground- and excited-state properties of the e_g-orbital degenerate Hubbard model at quarter filling for two kinds of lattices, zigzag chain and ladder. In the zigzag chain, the system is effectively regarded as a decoupled double chain of the S=1/2 antiferromagnetic Heisenberg model, and the spin gap is approximately zero, similar to the case of weakly coupled Heisenberg chains. On the other hand, in the ladder, the spin correlation on the rung remains robust and the spin gap exists.

Key words:
orbital degree of freedom, geometrical frustration, density matrix renormalization group method

Frustration among competing interactions is a key issue to bring richness of cooperative phenomena in magnetic systems [1]. For instance, antiferromagnets with the triangle-base structure possess frustration, since it is impossible to satisfy all the interactions. To suppress the effect of frustration, spins compromise with each other to take the noncollinear 120° structure. On the other hand, when electrons partially fill degenerate orbitals, it is necessary to consider the orbital as an internal degree of freedom in addition to the spin. The spatial anisotropy of the orbital causes electron hopping between orbitals depending on the direction, hence it is important to take account of the lattice geometry to understand the spin-orbital structure even in a simple cubic lattice. In particular, it is interesting to consider the effect of the orbital anisotropy on the frustrated lattice.

In this paper, we investigate the e_g-orbital degenerate Hubbard model at quarter filling on the zigzag chain and the ladder. When the Hund's rule coupling J is small, it is found that the ground state is a paramagnetic (PM) phase with ferro-orbital (FO) ordering. Here we focus on the PM phase and set J=0 for simplicity. The effect of J will be discussed elsewhere in the future. Then, the Hamiltonian is given by

$$H = \sum_{\mathbf{i},\mathbf{a},\gamma,\gamma',\sigma} t^{\mathbf{a}}_{\gamma\gamma'} d^{\dagger}_{\mathbf{i}\gamma\sigma} d_{\mathbf{i}+\mathbf{a}\gamma'\sigma} + U \sum_{\mathbf{i},\gamma} \rho_{\mathbf{i}\gamma\uparrow}\rho_{\mathbf{i}\gamma\downarrow} + U' \sum_{\mathbf{i},\sigma,\sigma'} \rho_{\mathbf{i}a\sigma}\rho_{\mathbf{i}b\sigma'}, \quad (1)$$

where $d_{\mathbf{i}a\sigma}$ ($d_{\mathbf{i}b\sigma}$) is the annihilation operator for an electron with the spin σ in the $d_{3z^2-r^2}$ ($d_{x^2-y^2}$) orbital at the site $\mathbf{i}$, $\rho_{\mathbf{i}\gamma\sigma}$=$d^{\dagger}_{\mathbf{i}\gamma\sigma} d_{\mathbf{i}\gamma\sigma}$, and $\mathbf{a}$ is the vector connecting adjacent sites. Note that the lattices are arranged in the (x, y)-plane as shown in Fig. 1. The hopping amplitudes are given by $t^{\mathbf{x}}_{aa}$=$t/4$, $t^{\mathbf{x}}_{ab}$=$t^{\mathbf{x}}_{ba}$=$-\sqrt{3}t/4$, $t^{\mathbf{x}}_{bb}$=$3t/4$ for the x-direction, $t^{\mathbf{y}}_{aa}$=$t/4$, $t^{\mathbf{y}}_{ab}$=$t^{\mathbf{y}}_{ba}$=$\sqrt{3}t/4$, $t^{\mathbf{y}}_{bb}$=$3t/4$ for the y-direction, and $t^{\mathbf{u}}_{aa}$=$t/4$, $t^{\mathbf{u}}_{ab}$=$t^{\mathbf{u}}_{ba}$=$\sqrt{3}t/8$, $t^{\mathbf{u}}_{bb}$=$3t/16$ along the zigzag path. Hereafter, t is taken as the energy unit. We employ the density matrix renormalization group method with the finite-system algorithm [2], which allows us to investigate the frustrated system with high accuracy. Here we consider each orbital as a virtual site to reduce the size of the superblock Hilbelt space. The number of states kept

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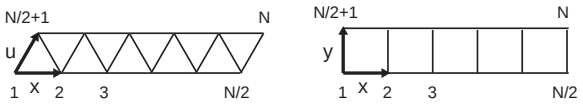

Fig. 1. Lattice configurations and numbering of the site. The zigzag chain and the ladder are considered as two-chain systems with the zigzag path and the rung, respectively.

for each block m is up to m=200 and the truncation error is estimated to be 10^{-5} at most.

In the strong-coupling region, each site is occupied by one electron, indicating that only spin and orbital degrees of freedom remain effective. In Fig. 2(a), the spin correlation function $C_{\rm spin}(\mathbf{i},\mathbf{j})=\langle S^z_{\mathbf{i}} S^z_{\mathbf{j}}\rangle$ with $S^z_{\mathbf{i}}=\sum_\gamma(\rho_{\mathbf{i}\gamma\uparrow}-\rho_{\mathbf{i}\gamma\downarrow})/2$ is shown for U=U'=20. In the zigzag chain, we find that the antiferromagnetic (AFM) correlation exists between intra-chain sites in each of a double chain, while the spin correlation between inter-chain sites is much weak. The double-chain spin structure is understood from the FO structure. In order to characterize the orbital shape, it is useful to define an angle $\theta_{\mathbf{i}}$ at each site as

$$\tan\theta_{\mathbf{i}} = \langle T^x_{\mathbf{i}}\rangle / \langle T^z_{\mathbf{i}}\rangle \qquad (2)$$

in the spirit of the mean-field approximation [3], where $T^x_{\mathbf{i}}=\sum_\sigma(d^\dagger_{\mathbf{i}a\sigma}d_{\mathbf{i}b\sigma}+d^\dagger_{\mathbf{i}b\sigma}d_{\mathbf{i}a\sigma})/2$ and $T^z_{\mathbf{i}}=\sum_\sigma(d^\dagger_{\mathbf{i}a\sigma}d_{\mathbf{i}a\sigma}-d^\dagger_{\mathbf{i}b\sigma}d_{\mathbf{i}b\sigma})/2$. By using $\theta_{\mathbf{i}}$, the new operators are defined as $\tilde{d}_{\mathbf{i}a\sigma}=e^{i\theta_{\mathbf{i}}/2}[\cos(\theta_{\mathbf{i}}/2)d_{\mathbf{i}a\sigma}+\sin(\theta_{\mathbf{i}}/2)d_{\mathbf{i}b\sigma}]$ and $\tilde{d}_{\mathbf{i}b\sigma}=e^{i\theta_{\mathbf{i}}/2}[-\sin(\theta_{\mathbf{i}}/2)d_{\mathbf{i}a\sigma}+\cos(\theta_{\mathbf{i}}/2)d_{\mathbf{i}b\sigma}]$ [4], which determine the orbital shape. For the zigzag chain, $\theta_{\mathbf{i}}\simeq 4\pi/3$ is observed, indicating the $(3x^2-r^2)$-type FO structure shown in Fig. 2(b). The orbital shape extends along the double chain, not along the zigzag path, to gain the kinetic energy by electron hopping. Namely, the AFM superexchange interaction along the u-direction J_1 is much weaker than that along the x-direction J_2. Note that J_2/J_1 is estimated to be 64^2 for the $(3x^2-r^2)$-type FO structure. Thus, due to the orbital anisotropy, the spin correlation along the zigzag path is weakened to suppress the effect of frustration. On the other hand, the spin correlation on the rung remains robust in the ladder, since the orbital shape extends to both the leg- and rung-directions, as shown in Fig. 2(c).

In order to consider how the orbital state is affected by the spin excitation, we investigate the orbital shape in the lowest-energy state with $S^z_{\rm tot}$=1, where $S^z_{\rm tot}$ is the z-component of total spin. In the zigzag chain, the FO structure with the same orbital shape as that in the ground state is observed. Namely, the double-chain nature remains even in the spin-excited state. Thus, it is expected that the spin excitation should be described by the zigzag spin chain with large J_2/J_1. For the zigzag spin chain, it has been found that the spin gap decreases exponentially with increasing J_2/J_1 [5]. In Fig. 2(d), the system-size dependence of the spin gap is shown. We find that the spin gap converges to almost

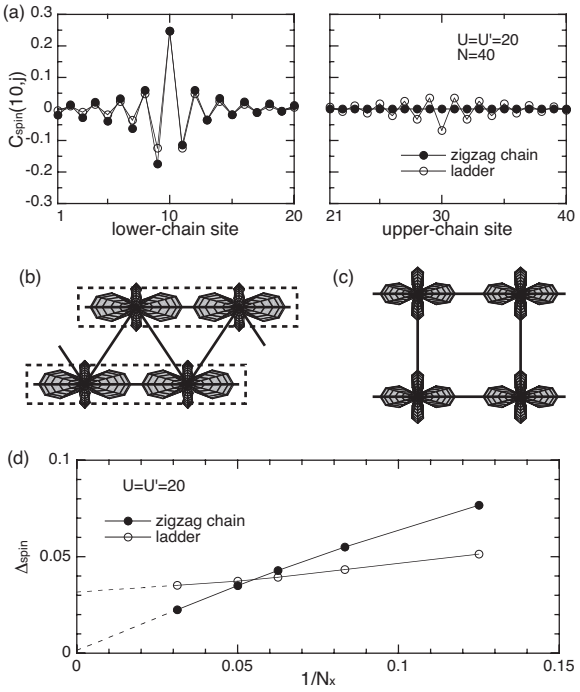

Fig. 2. (a) The spin correlation functions for the lower- and upper-chains from the center of the lower chain in the PM ground state. The FO structures for (b) the zigzag chain and (c) the ladder. (d) The spin gap vs. $1/N_x$ with N_x=$N/2$. The dotted line denotes the linear extrapolation to N_x=∞.

zero in the thermodynamic limit, as expected by analogy with the zigzag spin chain. On the other hand, the FO structure occurs also in the ladder, although the orbital shape slightly changes from that in the ground state. A finite spin gap is observed in the ladder, as shown in Fig. 2(d). Details of the spin-orbital structure in the spin-excited state will be discussed elsewhere.

In summary, the zigzag chain is effectively decoupled to two chains by orbital ordering to suppress the effect of frustration. Accordingly, the spin gap is approximately zero in the zigzag chain, while a finite spin gap exists in the ladder.

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